# Light-Duty Diesel Combustion

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**Project ID: ACS002**

# Overview

## Timeline:

Project started in 1997 to support DOE/OEM advanced engine development projects

Continuous evaluation of direction through frequent OEM feedback

## Budget:

Funded by DOE on a year-by-year basis

- SNL: $885k (*original FY17 budget*)
  - PI, post-doc, technologists, lab costs
- UW: $113k subcontract
  - 50% post-doc

## VTO program: barriers addressed

**A:** Lack of fundamental knowledge of advanced engine combustion regimes

**B, G:** Lack of cost-effective emission control

**C:** Lack of modeling capability for combustion and emission control

## VTO program: technical targets addressed

40% fuel economy improvement over 2009 baseline gasoline vehicle

Tier 2, bin 2 emissions

Emission control efficiency penalty <1%

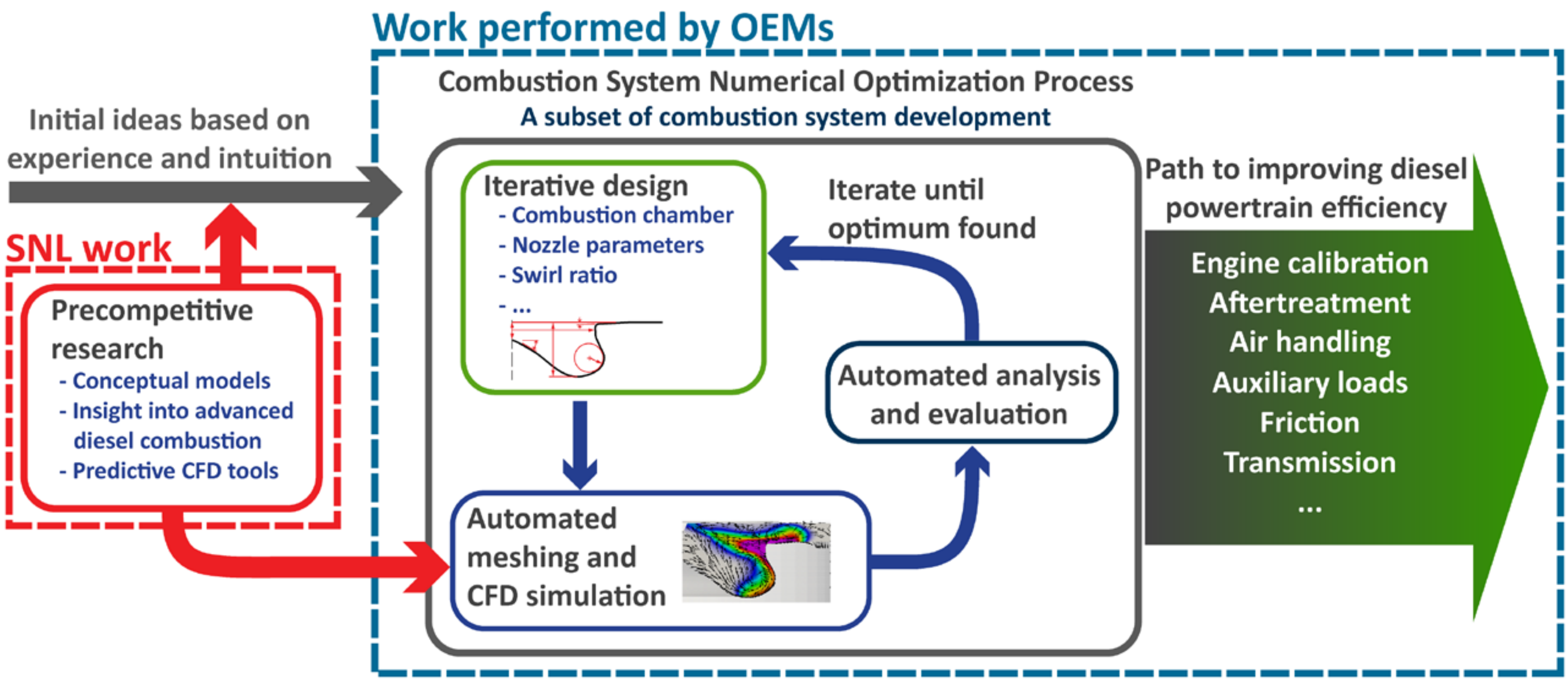
Specific cost: $30/kW

## Partners:

| | GM | Ford | UW (Reitz-Perini) | UW (Kokjohn) | ORNL (ACS016) | ANL | CSI | SNL (Pickett/Skeen) |
|---|---|---|---|---|---|---|---|---|
| Frequent discussion of results | ■ | ■ | ■ | | | | ■ | |
| Optical data exchange for code eval | | | ■ | | | | ■ | |
| Informal exchange of data and ideas | | | | ■ | | | | |
| Direct input on project directions | ■ | ■ | | | | | | |
| Lending of common rail hardware | ■ | | | | | | | |
| Direct collaboration (in planning) | | | | | ■ | ■ | | ■ |
| Direct collaboration (ongoing) | | | | | ■ | ■ | | |

# Relevance of precompetitive light-duty diesel research

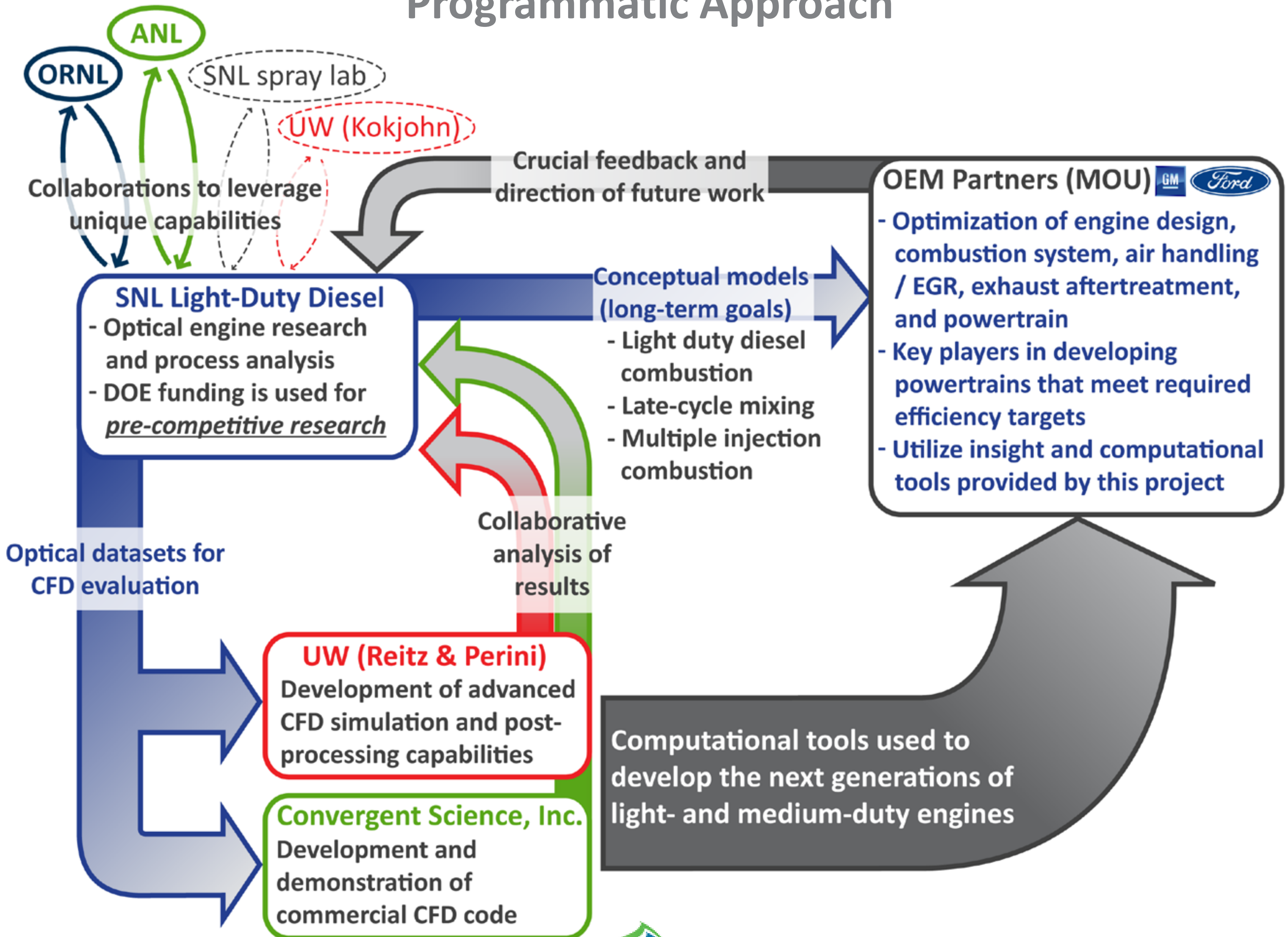
- Precompetitive research supports the development of advanced, fuel efficient diesel powertrains in two ways:
  - Provides OEMs with a science-based understanding of advanced diesel combustion as they develop and analyze combustion system concepts and calibrate engines
  - Developing more accurate predictive CFD tools for numerical optimization processes



# Relevance of studying piston bowl geometry

- Piston bowl geometry directly affects thermal efficiency and emissions
  - The physical mechanisms responsible for bowl geometry impacts on combustion and efficiency are not well documented
  - CFD predictions of a combustion system's response to a bowl geometry change have not been verified with experimental / optical data
- An experimental and computational study of bowl geometry impacts will:
  - Provide insight into mechanisms responsible for thermal efficiency and emissions improvements resulting from a change in combustion chamber geometry
  - Support development and evaluation of improved CFD tools to accurately predict combustion system response to a change in piston bowl geometry
- Activities in this review period
  - SNL: generate optical datasets to characterize liquid fuel injection, mixture formation, and combustion processes with two production-like piston geometries
  - UW: implement fuel injection / spray models in the FRESCO CFD platform; evaluate turbulence modeling using ECN data; compare simulations with experimental data
  - Provide insight into how bowl geometry impacts in-cylinder turbulent flow structures and mixing behavior

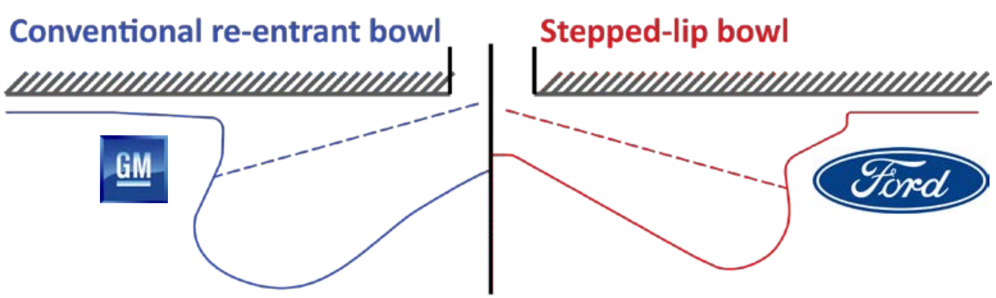
# Programmatic Approach



# Technical Approach

## Example: piston geometry study

- Adapt two piston geometries from production engines that represent two competing approaches
- Generate thermodynamic and optical datasets for each piston to characterize flow, mixing, combustion, and pollutant emissions
  - Analyze engine data to understand differences in combustion system behavior
- Corresponding CFD simulations for both piston geometries (UW)
  - Develop and evaluate state-of-the-art modeling capabilities to predict combustion system performance: <u>trends and phenomenology first; quantitative results second</u>
  - Develop advanced post-processing techniques to extract additional insight about in-cylinder processes and support experimental findings



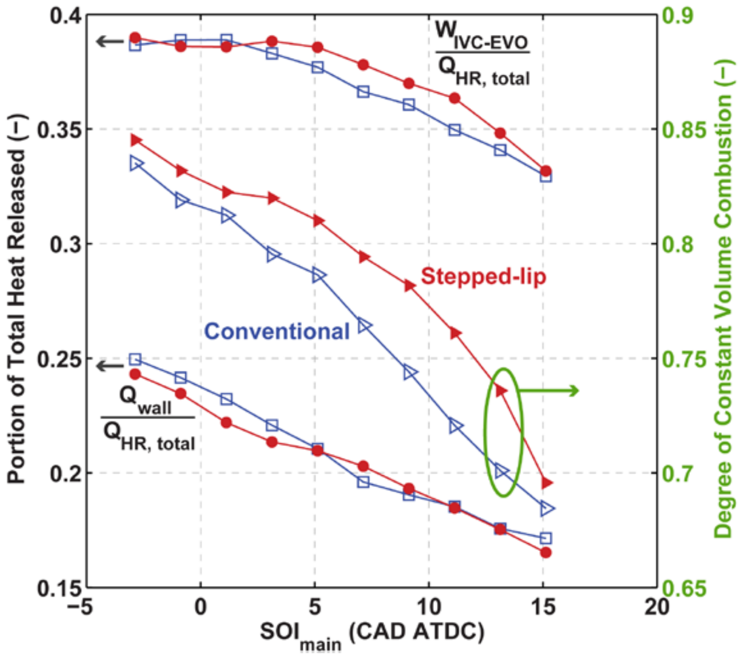

- Closely resembles GM 1.9L bowl geometry
- Spray targeting based on GM guidance

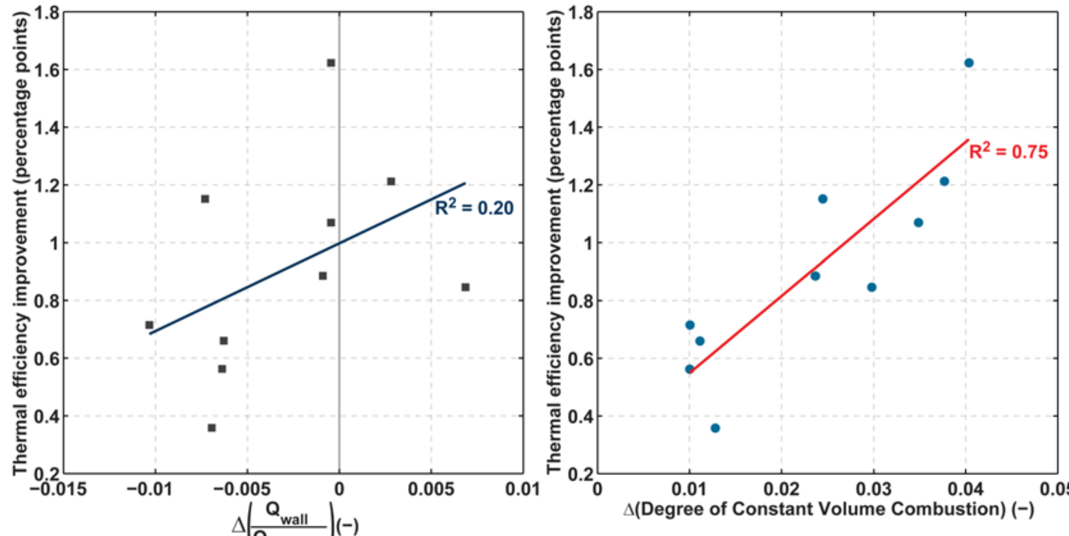
- Scaled version of Ford 6.7L bowl geometry
- Spray targeting based on Ford guidance

RANS-based CFD simulations for this study are performed under subcontract at the University of Wisconsin using the FRESCO CFD platform. See backup slides for details about models used for this work.

# TA: First-law thermodynamic analysis provides insight into efficiency advantages with a stepped-lip piston

Faster late-cycle heat release increases the degree of constant volume combustion and thereby thermal efficiency; changes in late-cycle mixing due to bowl geometry directly influence thermal efficiency.




Wall heat loss can be reduced with the stepped-lip bowl, but the largest efficiency differences do not correlate with the largest differences in wall heat loss

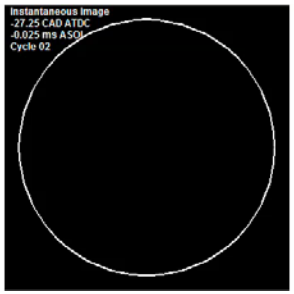
$$\eta_{CV} = \frac{1}{\eta_{Otto} Q_{HR}} \int 1 - \left(\frac{V_h + V_c}{V(\theta)}\right)^{1-\gamma} \frac{dQ_{HR}}{d\theta} d\theta$$

- Wall heat loss changes are not correlated with thermal efficiency changes
- An increased degree of constant volume combustion bowl correlates more strongly with thermal efficiency improvement
  - Faster late-cycle mixing is responsible for a higher degree of constant volume combustion
  - Late-cycle mixing is influenced by bowl geometry and directly impacts thermal efficiency

# TA: time-resolved liquid scattering imaging data has been used to evaluate CFD simulation capabilities to predict liquid fuel behavior

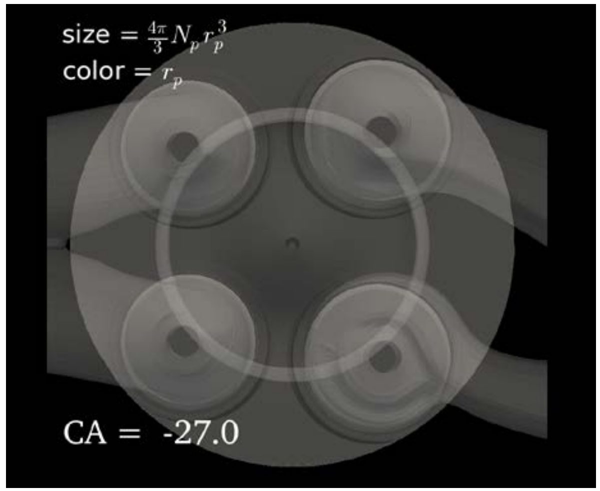
**SNL** high speed imaging data

-distortion corrected



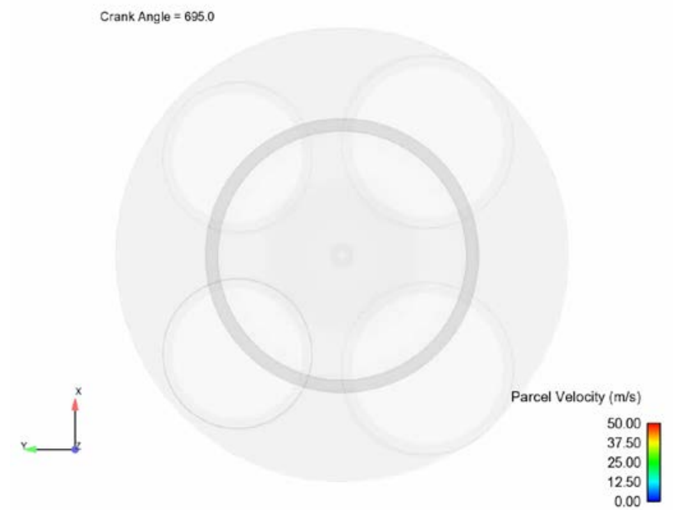

**FRESCO** simulation results (UW)

-spray models calibrated with ECN data

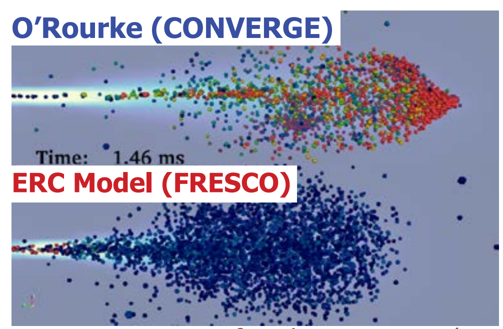



**CONVERGE** simulation results

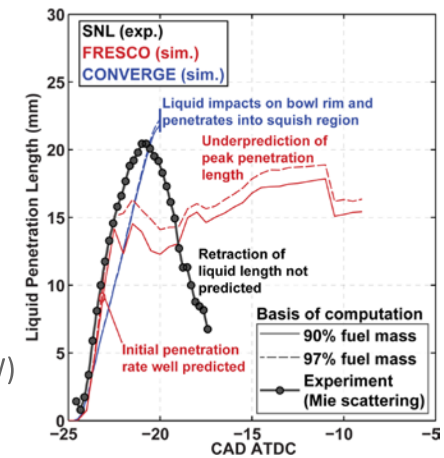
-spray models calibrated with ECN data




- High speed Mie scattering data has been collected and processed at SNL to characterize liquid fuel behavior for a main-only injection strategy (LTC operation, DPRF fuel)
- The CONVERGE simulations consistently over predict liquid penetration and incorrectly predict liquid impingement on the bowl rim
- Choice of droplet coalescence model* may be critical to accurate prediction of liquid behavior




Images courtesy of Federico Perini (UW)

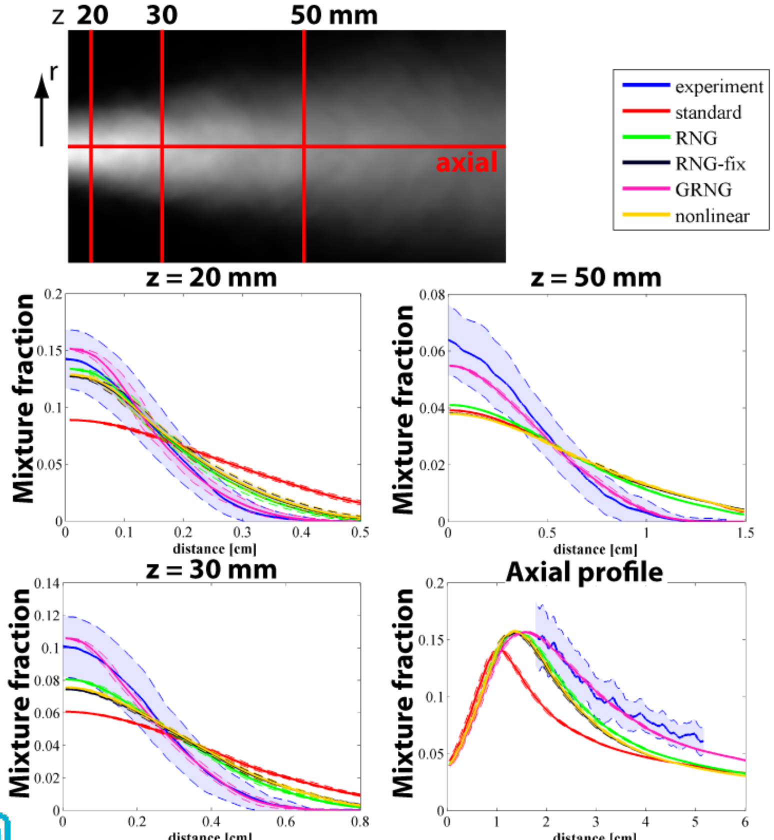



*See backup slide for modeling details

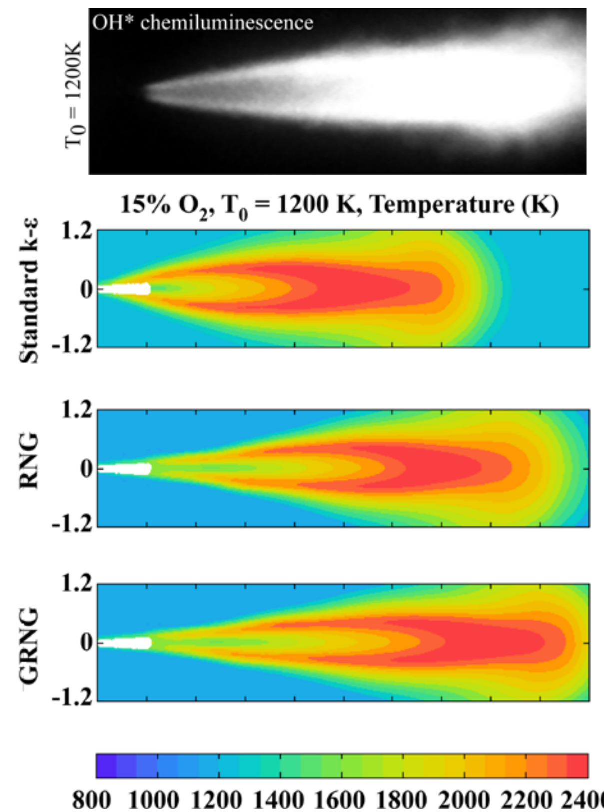
# TA: Spray models have been calibrated using ECN spray A data and multiple two-equation turbulence models have been evaluated using FRESCO

The Generalized RNG (GRNG) turbulence model (a product of SNL-UW collaboration) has been determined to produce the best accuracy trade-off between cold engine flow and jet flow / spray combustion based on comparisons with state-of-the-art ECN data.

## Mixture formation is better predicted with the GRNG turbulence model

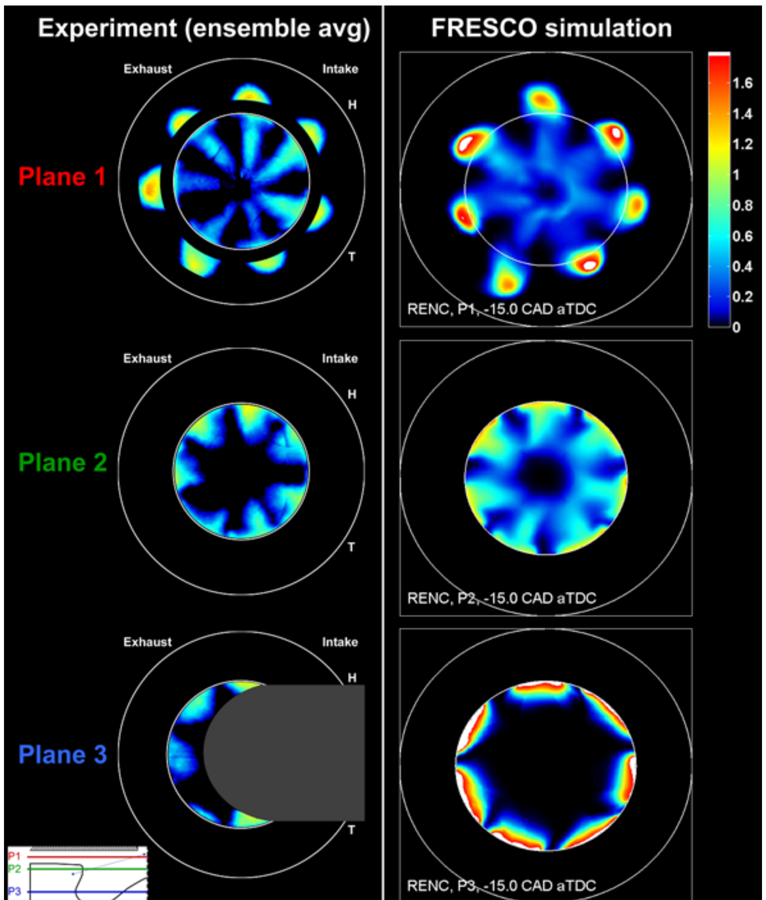



## The GRNG model yields the most accurate flame structure predictions

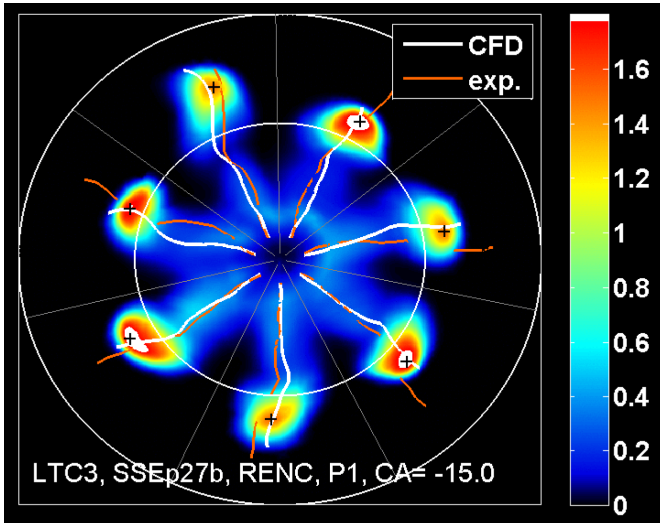


# TA: quantitative fuel tracer concentration data (SNL) have been used to evaluate FRESCO's ability to predict vapor behavior and spray-swirl interactions

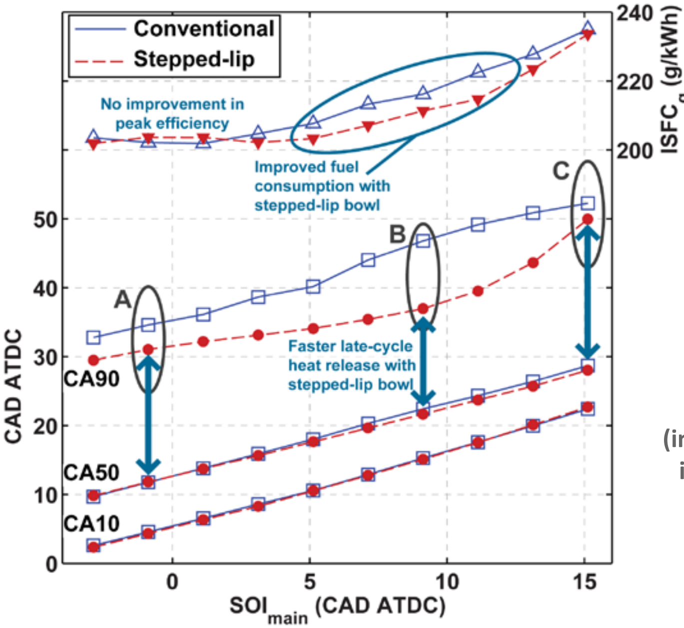
- Quantitative fuel tracer PLIF data has been generated by SNL to evaluate CFD simulations
  - True test of FRESCO's predictive capability: no tuning of spray models after calibration with ECN data
  - Multiple comparison metrics have been computed from both experimental and simulation results
- Overall vapor penetration behavior is well predicted
- Jet-swirl interactions are faithfully predicted

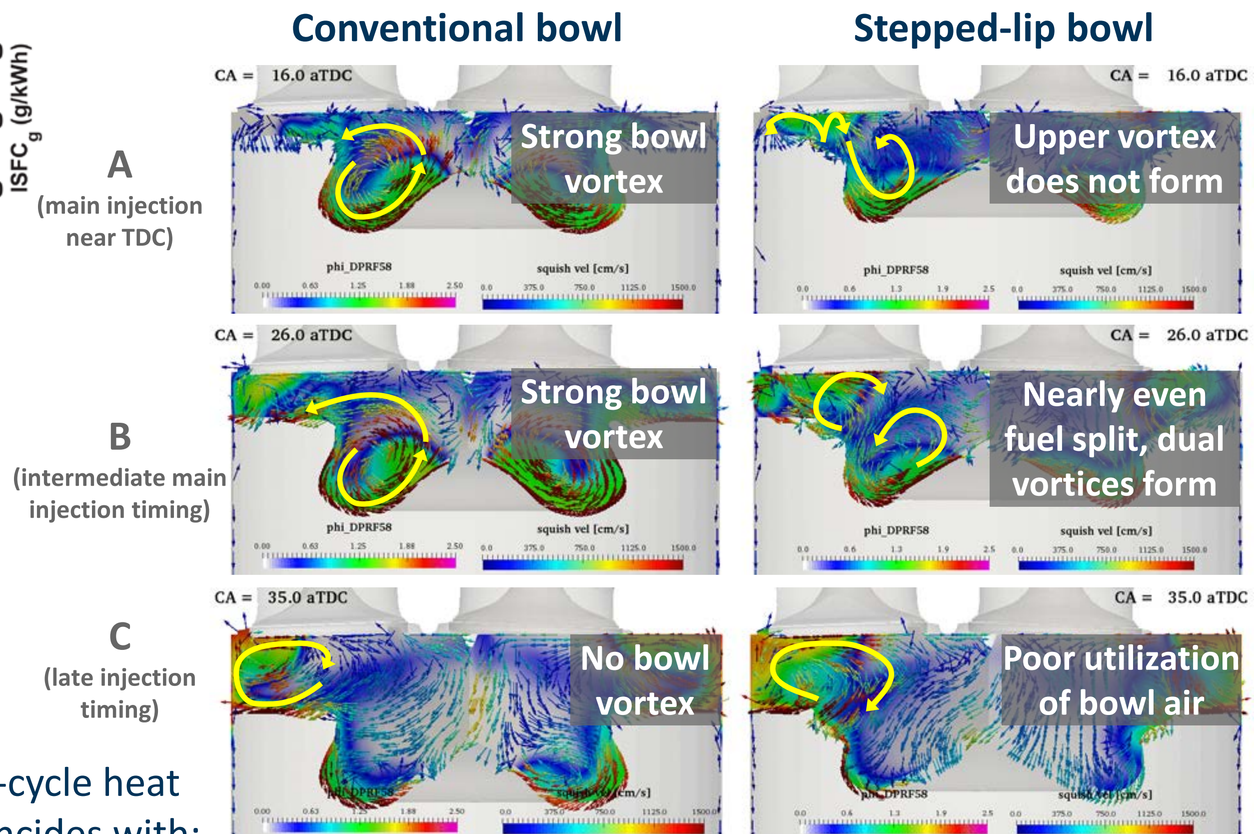



The unsteady gas-jet model used in the FRESCO simulations reliably captures the momentum exchange between the sprays and squish/swirl flows



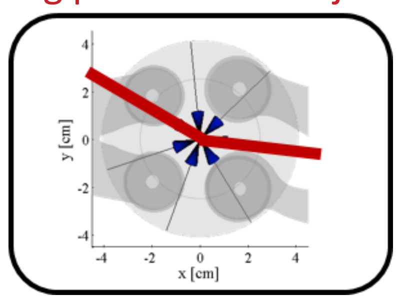
# TA: FRESCO CFD simulations provide insight into the effects of bowl geometry and injection timing on vortex dynamics




- Simulation results show faster late-cycle heat release in the stepped-lip bowl coincides with:
  - Effective fuel splitting at the step
  - Formation of dual toroidal vortices
- Vortex dynamics, fuel splitting, and the associated air utilization improvement may be key to increasing peak thermal efficiency

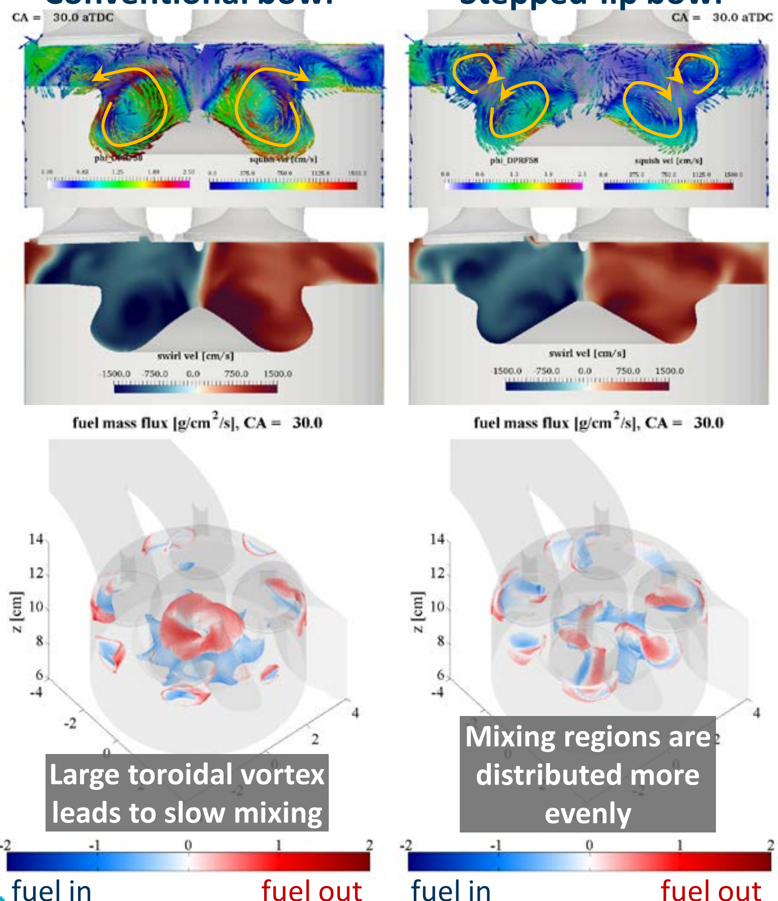
Cutting planes contain jet axes

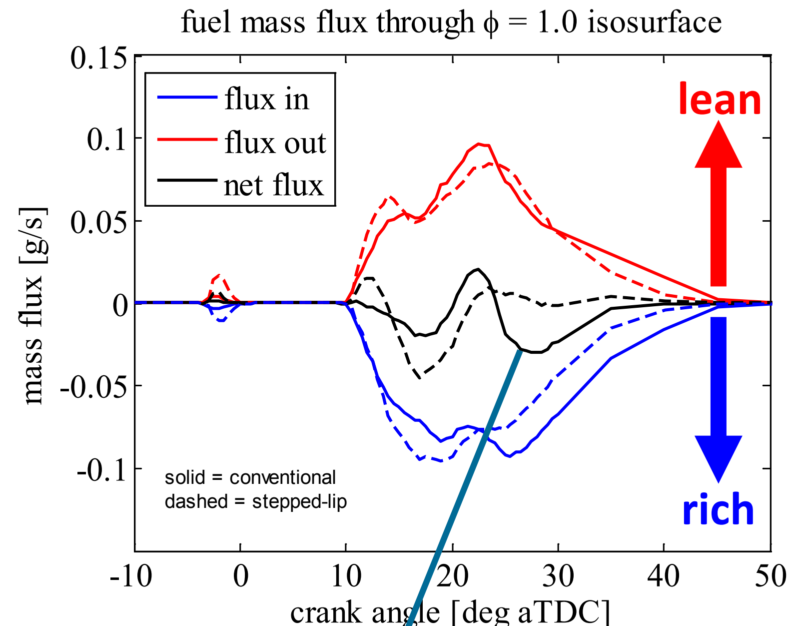


# TA: CFD results predict rich mixtures persisting in the conventional piston bowl; experimental results are consistent with the CFD prediction

- Advanced post-processing techniques have been developed to provide insight into mixing processes predicted by FRESCO CFD simulations

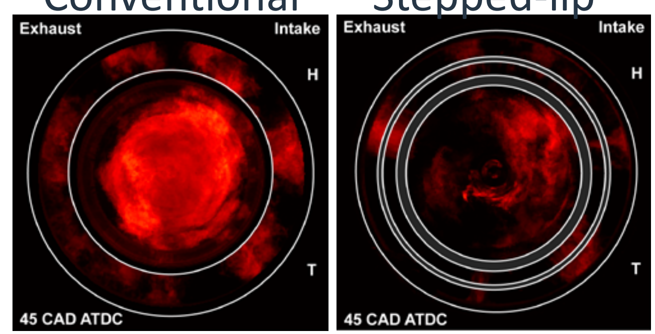
**Conventional bowl** **Stepped-lip bowl**




**Richer conditions persist longer in the conventional bowl; natural luminosity images show a large amount of soot above the conventional bowl late in the cycle**

Conventional Stepped-lip



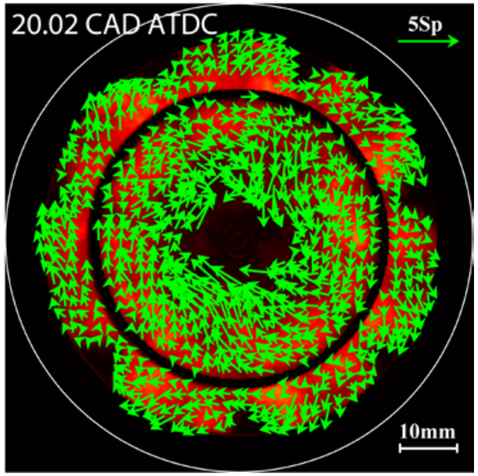
## Chemical kinetic mechanisms remain a research need and a source of uncertainty

- Attempts to simulate engine combustion using FRESCO with a reduced mechanism for DPRF (hexadecane + 2,2,4,4,6,8,8-heptamethylnonane) were unsuccessful
  - Sprays do not ignite under any of the simulated engine conditions
- A well-tested reduced DPRF mechanism does not yet exist for use in engine simulations
- A PRF (isooctane, n-heptane) reduced kinetics model may be adequate for conventional diesel combustion conditions
  - PRF25 has previously been used to approximate DPRF58 at intermediate and high temperatures with rich and stoichiometric mixtures
  - Low temperature behavior of PRF does not match the behavior of DPRF; ignition phenomena are not expected to be accurately predicted
- Simulation work is proceeding with a reduced PRF mechanism, but a reliable reduced DPRF mechanism is desired

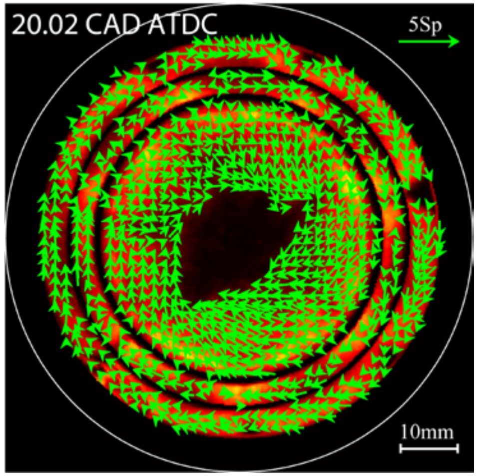
# TA: high speed natural luminosity imaging with both the conventional and stepped-lip pistons yields information about late-cycle flow patterns

- Late-cycle mixing is difficult to measure with laser-based planar techniques (PIV)
  - Laser sheet provides very limited access in the bowl
  - High soot concentrations → rapid laser extinction
- Combustion image velocimetry (CIV)
  - Utilizes high-speed natural luminosity (NL) images – easy to collect large datasets
  - Movement of coherent structures in the soot clouds is tracked as with PIV
  - Line-of-sight technique: interpretation of images is difficult and uncertainties can be large
  - Semi-quantitative results can be expected to indicate flow patterns above the bowl
  - Comparison with CFD requires post-processing techniques to be developed
- High speed NL imaging has been performed with both piston bowl geometries; images have been processed using CIV techniques (labor intensive)
  - Ongoing analyses will provide a **description of late-cycle flow patterns** with both piston geometries and facilitate **comparison with fired CFD results**

Sample data (conventional bowl)




Sample data (stepped-lip bowl)



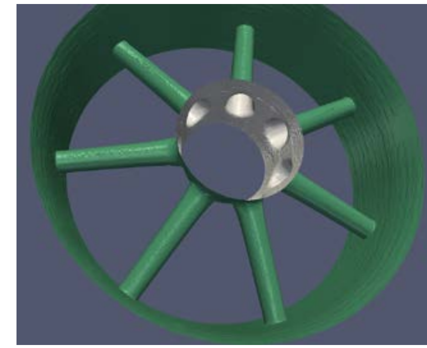
# TA: a new high pressure fuel delivery system has been designed and built at SNL to provide 3000+ bar injection pressure

- Previous fuel system (1997-2017)
  - Maximum pressure: 1220 bar
  - Aging components
  - Risk of fuel contamination
- New fuel system (2017-)
  - Maximum pressure: 3000+ bar
  - Currently configured with a new 2000 bar rail*
  - Pneumatic pump with automatic pressure control and safety monitoring
  - Minimal risk of fuel contamination
  - Shakedown testing in progress

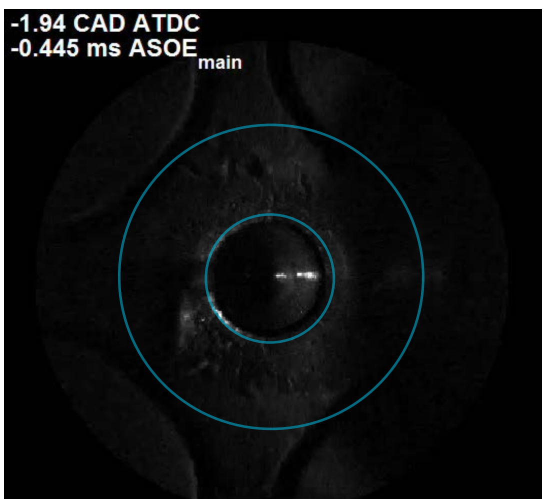
*We thank General Motors for generously providing new common rail hardware for this system

# TA: for the 7-hole solenoid injector used for light-duty multiple injection studies, jet-to-jet variability cannot be attributed to hole-to-hole variation in the nozzle

- Full spectrum x-ray tomographic imaging has been performed at the Advanced Photon Source at Argonne National Laboratory to investigate SNL's 7-hole injector
- Analysis at ANL indicates minimal hole-to-hole variation
  - Diameter, radius of curvature, and eccentricity: highly repeatable
- Liquid and vapor-phase fuel imaging at SNL indicates significant jet-to-jet variability in spreading angle and penetration length
  - This variability cannot be explained by nozzle geometry
  - Internal nozzle flow is likely responsible for jet-to-jet variability

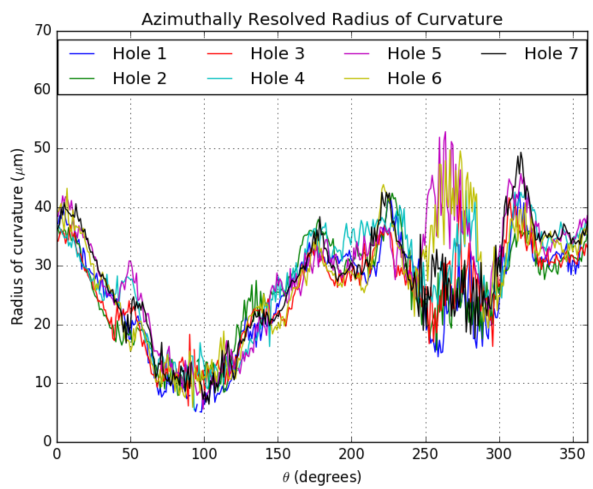


## Liquid fuel imaging (SNL)

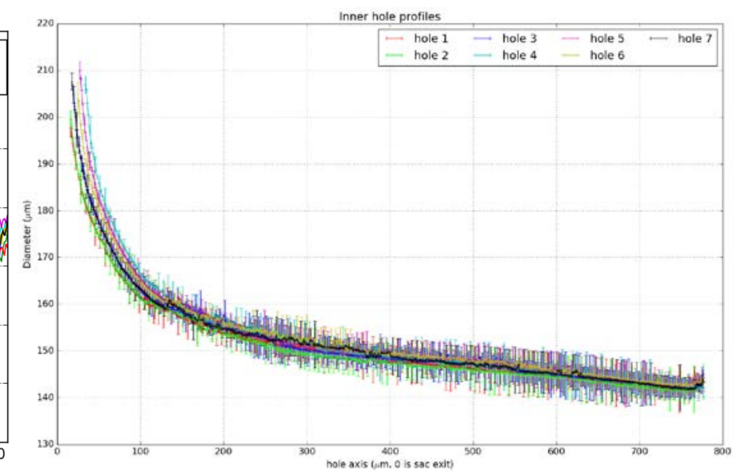



Circles shown for reference.

## Radius of inlet curvature (ANL)



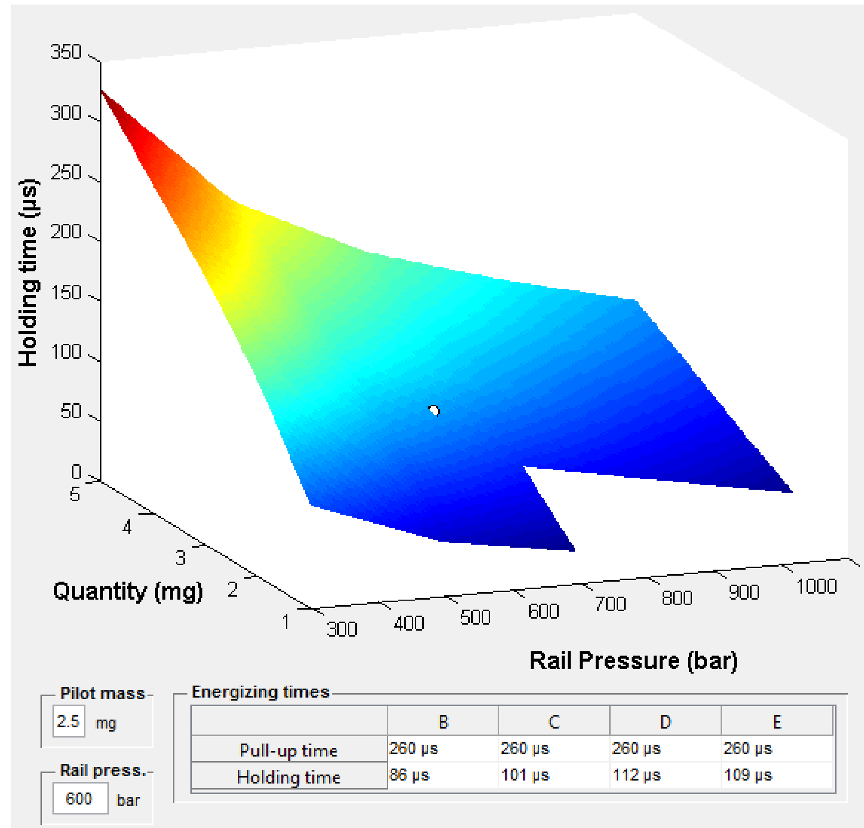

## Inner hole diameter profiles (ANL)




Chris Powell and Katie Matusik at ANL are gratefully acknowledged for performing the high-resolution tomographic x-ray imaging and analyzing the geometric data

# TA: project plan developed to investigate tradeoffs between efficiency and combustion noise at ORNL; initial injector characterization completed

- Project concept and statistical experiment design completed (SNL)
  - Goal: characterize tradeoffs between efficiency and combustion noise at constant load
    - LTC and conventional operation
    - Impact of close-coupled pilots
  - Critical input on project motivation and approach provided by Eric Kurtz (Ford)
- Initial characterization of common rail injectors (donated to SNL by Delphi) has been completed at SNL
  - Given rail pressure, cylinder pressure, and desired pilot mass, the corresponding solenoid energizing times are now known for each injector



# Responses to reviewers

**The work underway is far from making any real impact on the merits of LD diesels in the United States. Will the work the team is doing invite manufacturers towards the introduction of LD diesels to the U.S. in the next 20 years?**

Understanding how bowl geometry affects late-cycle mixing and thermodynamic efficiency, as well as developing the capability to predict combustion system response to bowl geometry changes, are essential for the development of the next generation of light-duty diesel engines. Future work with catalyst heating operation will provide fundamental understanding of calibration sensitivities for a challenging operating regime.

**The project would merit a great deal with active participation from an OEM that is committed to the LD diesel product in the United States. A committed OEM may be able to provide a more focused approach to the current work.**

We are fortunate to work very closely with GM and Ford to share the findings of our work and to develop our future project plans through regularly scheduled teleconferences and face-to-face meetings. We have engaged FCA and invited their diesel R&D team (in Italy) to participate more actively in the AEC MOU, and we welcome collaborations with any other OEMs who may be interested.

**The project has been in development for a long time. What timeline do the PIs envision before work will be completed?**

Building conceptual models of light-duty diesel combustion, piloted diesel combustion, and late-cycle oxidation behavior will require years of sustained research and analysis. The development of truly CFD predictive models requires better understanding of sprays and atomization processes, and chemistry remains a large uncertainty source. These very significant research challenges seem unlikely to be resolved within a decade. We will continue to carefully consider this question as we develop new projects to help us toward our goals.

**Are FRESCO/RAPTOR open-source, or will they become open-source?**

Supporting an open-source community is extremely resource intensive. For this reason, RAPTOR cannot be supported as an open-source code. FRESCO is intended to become an open-source platform for engine research but this goal is dependent on resource availability.

**Will FRESCO be used to investigate soot formation? What diagnostics will be employed in the experiments and what strategies are proposed if the model does not match the data?**

We plan to use the FRESCO platform to study soot formation/oxidation. Please see the backup slides for more detail about our intended approach.

**Does FRESCO have the capability to deal with multicomponent liquid fuel effects?**

FRESCO currently employs a full multi-component liquid vaporization model; the binary mixtures used in engine experiments are directly modeled. Future plans include a full phase equilibrium-based approach that has recently been developed at UW. See backup slide for more detail.

**Exploring an optimized piston geometry, either experimentally via rapid hardware prototyping or via CFD, must be part of future work.**

Combustion chamber geometry optimization is competitive work. One of our goals as a national lab is to help develop, validate, and publish CFD modeling approaches used to accurately predict combustion system response to a known change in bowl geometry. OEMs will use advanced CFD models within their combustion system development processes to find optimal nozzle parameters, swirl levels, new bowl geometries, etc.

**Indicated efficiency results do not relate directly to DOE goals; metal engine work at ORNL is one way to accomplish this.**

Fuel economy improvements ultimately depend on engine development and calibration work by OEMs. We help them build more efficient engines by providing them with scientific understanding and tools to predict combustion system design and calibration parameter impacts on efficiency and emissions. OEMs are experts on tradeoffs between efficiency, noise, emissions, and aftertreatment, and they use improvements in fundamental understanding to improve powertrain efficiency.

# Future work

Any proposed future work is subject to change based on funding levels

- Piston bowl geometry study
  - CFD (UW): Addition of PRF kinetic mechanism to simulations; predictions of combustion and soot emissions
  - Comparison of CFD results with experimental CIV data, full analysis of soot and efficiency trends
  - Development of next set of experiments in collaboration with Ford and GM, if deemed valuable
- Pilot injection studies
  - Impact of low-temperature chemistry / turbulence interactions on main ignition with and without a pilot injection: continued development of formaldehyde LIF technique
  - Spectrographic imaging: understanding combustion luminosity after pilot heat release has finished
  - Impact of pilot-main dwell on main ignition for various swirl ratios
  - Building understanding to support long-term development of multiple injection conceptual models
- New collaborative project (ORNL-SNL): catalyst heating operation
  - Project concept developed in close collaboration with Ford and GM
  - Sources of formaldehyde/UHC emissions and engine calibration sensitivities with cat heating operation
  - Possibility to explore cetane number effects
  - Engine testing, FTIR characterization at ORNL; injection rate measurements and imaging experiments (including formaldehyde PLIF) at SNL; supporting CFD simulations at UW
- Noise-efficiency tradeoffs (ORNL-SNL collaboration)
  - Measurement campaign tentatively scheduled (late summer 2016)
- Continued collaboration with ANL: high resolution x-ray imaging
  - X-ray diagnostics of needle lift/wobble, internal flow, and near-nozzle behavior with multiple injections
- Close-coupled post injection study (longer term; in planning with GM)
  - How does post injection quantity/dwell affect soot emissions in the light-duty diesel engine? Is the mechanism sensitive to bowl geometry?
- Collaboration with Pickett/Skeen (SNL, ACS005): main ignition processes with pilot injections
  - Augment engine studies with precision optical experiments in the SNL injection chamber with single- and multihole injectors
- Sharing optical data from the light-duty engine in the framework of the ECN
  - Contingent on ability to share engine and piston geometry data; talks with GM/Ford ongoing
  - Foster CFD code/model development for engine applications

# Summary

## Relevance

- Pre-competitive research: necessary to develop scientific understanding of advanced diesel combustion and to develop / evaluate new CFD models used to design future diesel combustion systems
- Piston bowl design impacts efficiency and emissions; the underlying mechanism is not understood

## Approach

- SNL: optical light-duty diesel engine experiments, digital image processing, and combustion process analysis; adaptation of production piston designs for study in the optical engine
- UW (subcontract): using FRESCO CFD platform; model development and evaluation based on optical data, provide post-processed CFD results to supplement insights gained from optical measurements
- Close collaboration with GM and Ford to discuss results and determine future projects

## Technical Accomplishments

- Enhanced late-cycle heat release is largely responsible for efficiency improvements with a stepped-lip bowl
- Optical datasets acquired and processed at SNL: high-speed liquid fuel imaging, quantitative fuel concentrations, natural luminosity imaging / CIV; data shared with CFD partners (UW, CSI) for model evaluation purposes
- FRESCO CFD models have been calibrated using ECN data; the GRNG turbulence model is the best compromise; predictions of fuel injection and mixing behavior in the SNL light-duty diesel engine appear reasonable
- FRESCO simulations (non-combusting) suggest that thermal efficiency improvements with the stepped-lip bowl may result from enhanced fuel splitting and the formation of dual toroidal vortices

## Collaborations

- Strengthening collaborations with ORNL (Curran) and ANL (Powell)
- Continuing collaboration with Convergent Science
- Planned collaboration with Skeen/Pickett

## Future Work

- Continue to develop understanding of piston bowl geometry effects, pilot injection strategies
- Formaldehyde PLIF: ignition processes and sources of UHCs
- Catalyst heating operation: collaborative project (ORNL-SNL), concept developed together with Ford and GM

# Backup slides

# Measures required to improve light-duty diesel fuel economy

- Downsizing while maintaining equal power
  - Increased boost – two stage turbocharging
  - Higher injection pressures to increase specific power
  - Improved engine durability to support higher loads
- Reducing engine friction
  - Piston assembly friction is the largest friction source
- Reducing auxiliary loads
  - Electrically driven, switchable coolant pump
  - Dual-mode/modulated oil pump
  - Reduced fuel circulation
- Optimizing transmission
  - More gear ratios to maintain high efficiency over a wide range of speeds and road loads

Pertinent to research at SNL

- Improving thermodynamic efficiency
  - Enabling optimized engine calibrations through optimized combustion over the entire range of engine operation (much more than just peak efficiency improvements)
  - Demands better understanding of spray dynamics, swirl-spray-bowl interactions, chemical reactions, late-cycle mixing, pollutant formation, etc.

# How improvements in combustion processes impact fuel consumption

- Improvements in diesel thermal efficiency are expected to reduce light duty fuel consumption by approximately 3% between 2007 and 2020[1]
- Factors that influence gross indicated thermal efficiency (the closed portion of the cycle)
  - Combustion phasing (may be limited by emissions/noise/peak pressure constraints)
  - Combustion duration (influenced by injection strategy and bowl design)
  - Wall heat loss (also impacts exhaust enthalpy)
  - Specific heat ratio (relatively high for operation with excess air)
  - Compression/expansion ratios
- OEMs utilize improvements in tradeoff behavior to achieve more efficient engine calibrations
  - Increasing air utilization through improved combustion chamber geometry design is an effective method to improve the soot-$NO_x$ tradeoff

Example: soot emissions are reduced as a result of improved air utilization; the engine's EGR tolerance improves. Higher EGR levels mean that NOx emissions are reduced, and injection timing can be advanced to increase efficiency without exceeding NOx and soot emissions targets.

[1] Assessment of Fuel Economy Technologies for Light-Duty Vehicles", Committee on the Assessment of Technologies for Improving Light-Duty Vehicle Fuel Economy; Board on Energy and Environmental Systems; Division on Engineering and Physical Sciences; National Research Council; The National Academies Press, Washington, D.C., 2011.

# Turbulence and spray models used in CFD simulations

| Phenomenon | Model (FRESCO) | Calibration (FRESCO) | Model (CONVERGE) |
|---|---|---|---|
| **Turbulence** | GRNG (generalized re-normalization group) | Calibration not needed for jet flow | RNG k-epsilon model |
| **Spray atomization** | Lagrangian-particle/Eulerian-Fluid; hybrid KH-RT instability; Spray angle according to Reitz and Bracco | Significant calibration of the atomization process is needed: there are 7-8 parameters for each aspect of the breakup. A genetic algorithm has been applied to obtain an optimized set of model parameters using ECN data; no tuning is performed for engine testing | Lagrangian-particle/Eulerian-Fluid; blob injection model (initial drop sizes equal to effective nozzle diameter); O'Rourke turbulent dispersion model; dynamic drop drag model; KH-RT modified breakup model; spreading angle tuned for engine simulations |
| **SGS near-nozzle flow** | Unsteady gas-jet model with implicit momentum coupling | Does not require calibration | - |
| **Droplet collision** | Deterministic impact with extended outcomes, dynamic ROI (radius-of-influence) | Does not require calibration | NTC collision model with post model for collision outcomes |
| **Droplet vaporization** | Discrete multi-component, Torres | Does not consider real-gas effects, but does not need calibration | Frossling correlation to model spray evaporation; multicomponent vaporization |


For details about spray and turbulence models currently implemented in FRESCO, please see:

1. Perini, F. and Reitz, R. D., "Improved atomization, collision and sub-grid scale momentum coupling models for transient vaporizing engine sprays," International Journal of Multiphase Flow 79 (107-123), 2016, doi: http://doi.org/10.1016/j.ijmultiphaseflow.2015.10.009
2. Perini, F., Zha, K., Busch, S. and Reitz, R., "Comparison of Linear, Non-Linear and Generalized RNG-Based k-epsilon Models for Turbulent Diesel Engine Flows," SAE Technical Paper 2017-01-0561, 2017, doi: 10.4271/2017-01-0561

For details about the full phase-equilibrium models that will be implemented in FRESCO, please see:

2. Yue, Z., Hessel, R.P., and Reitz, R.D., "Investigation of real gas effects on combustion and emissions in internal combustion engines and implications for development of chemical kinetics mechanisms," accepted for publication in the International Journal of Engine Research, 2016
3. Qiu, L., Wang, Y., Jiao, Q., Wang, H., and Reitz, R.D., "Development of a Thermodynamically Consistent, Robust and Efficient Phase Equilibrium Solver and its validations," Fuel, Vol. 115, pp. 1-16, 2014, doi: 10.1016/j.fuel.2013.06.039, 2014